CORRELATION ENERGY OF MEAN-FIELD FERMI GASES

QUANTISSIMA

15. 8. 2022

CORRELATION ENERGY OF MEAN-FIELD FERMI GASES

Marcello Porta (SISSA)

Based on joint works with:

N. Benedikter, P.T. Nam, B. Schlein, R. Seiringer; C. Hainzl, F. Rexze

Outline

*) Introduction to many body QM, fermionic systems

*) Mean field regime, Hartree Fock th.

*) Correlation energy, RPA (main res.)

*) Bogoliubov transfo., bosonization

<u>Setting</u>: <u>N interacting</u> quan<u>tum</u> parts:

Wave fcn: $\Psi_N \in L^2(\mathbb{R}^{3N})$ (omit spin)

Identical particles: $|\Psi_N(x_1, \dots, x_N)| = |\Psi_N(x_{\pi(1)}, \dots, x_{\pi(N)})|$

<u>Bosons</u>: $\Psi_N(x_1, \dots, x_N) = \Psi_N(x_{\pi(1)}, \dots, x_{\pi(N)})$

<u>Fermions</u>: $\Psi_N(x_1, \dots, x_N) = \operatorname{sgn}(\pi)\Psi_N(x_{\pi(1)}, \dots, x_{\pi(N)})$

Example : Slater determinants $\psi_N \in L^2_a(\mathbb{R}^{3N})$

Given $(f_i)_{i=1}^N$ $f_i \in L^2(\mathbb{R}^3)$, $f_i \perp f_j$ if $i \neq j$

$\| f_i \|_2 = 1$

$$\psi_N(x_1, \dots, x_N) = \frac{1}{\sqrt{N!}} \sum_\pi (-1)^\pi f_{\pi(1)}(x_1) \cdots f_{\pi(N)}(x_N)$$

$$= \frac{1}{\sqrt{N!}} \det \left(f_i(x_j) \right)_{1 \le i,j \le N} \quad (\|\psi_N\|_2 = 1)$$

<u>Hamiltonian</u> : H_N on $L^2(\mathbb{R}^{3N})$

$$H_N = \sum_{j=1}^{N} \left(-\Delta_j + V_{ext}(x_j) \right) + \sum_{i<j}^{N} V(x_i - x_j)$$

E.g.: atom Hamiltonian

*) $V_{ext}(x_j) = - \dfrac{Z}{|x_j|}$ $\quad Z > 0$

*) $V(x_i - x_j) = \dfrac{1}{|x_i - x_j|}$ $\quad \left(e = -1 , \hbar = 1 \right)$

Natural questions :

*) Ground state energy ?

$$E_N = \inf_{\substack{\psi_N \in L^2_a(\mathbb{R}^{3N}) \\ \|\psi_N\|_2 = 1}} (\psi_N, H_N \psi_N)$$

*) Excited states ?

*) Dynamical prop ? $\quad i\partial_t \psi_{N,t} = H_N \psi_{N,t}, \quad \psi_{N,0} \in L^2_a$

Difficulty : $N \gg 1$ $(N \to \infty)$

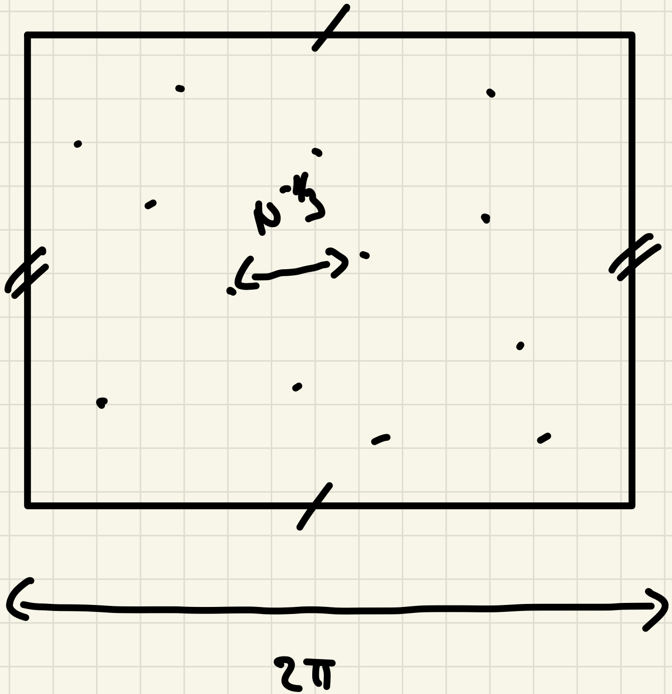
impossible to find exact sol., then find principles.

*) Effective theories : "simpler models", less deg. of freedom, "correct" as $N \to \infty$

Typically, nonlinear models.

*) We will focus on the mean field regime.

Mean field regime. "Coincidence of high density"



$(\mathbb{T}^3)$

N particles

$(N \gg 1)$

$|\Lambda| = (2\pi)^3$

$\rho = \frac{N}{|\Lambda|} = O(N) \gg 1$

Rmk: $\mathrm{dist}(i,j) \sim N^{-1/3}$

Hamiltonian: on $L^2_a(\mathbb{T}^{3N})$,

$$H_N = \sum_{j=1}^{N} -\Delta_j + \lambda \sum_{i<j}^{N} V(x_i - x_j)$$

*) $V(x_i - x_j)$ is N independent

" $\lambda \sum_{i<j}^{N} V(x_i - x_j) \sim \lambda N^2$ " (V bd)

*) Mean field: choose $\lambda = \lambda(N)$ s.t.

kinetic en. "$\simeq$" int. energy.

Kinetic energy.

*) To define, consider bosons:

$$\Psi_N = \varphi^{\otimes N} \quad (\text{condensate state})$$

$$\Big(\Psi_N, \sum_{j=1}^{N} -\Delta_j \Psi_N\Big) = N(\varphi, -\Delta\varphi) = \mathcal{O}(N)$$

*) Not true for fermions: particles cannot occupy the same state!
(Pauli principle)

Fermions : Consider a Slater determinant

$$\psi_N = \frac{1}{\sqrt{N!}} \sum_\pi (-1)^\pi f_{\pi(1)} \otimes f_{\pi(2)} \cdots \otimes f_{\pi(N)}$$

$(f_i, f_j) = \delta_{ij}$. Then,

$$\langle \psi_N, \sum_{j=1}^N -\Delta_j \psi_N \rangle = \sum_{j=1}^N (f_j, -\Delta_j f_j)$$

(exercise)

Suppose $f_i \in L^2(\mathbb{T}^3)$, eigenvectors of $-\Delta$

*) $f_i \longrightarrow f_{p_i}(x) = e^{ip_i x}/(2\pi)^{3/2}$

$p_i \in \mathbb{Z}^3 \qquad p_i \neq p_j \quad i \neq j.$

$-\Delta f_p = |p|^2 f_p$

*) $\left(\sum_{j=1}^N -\Delta_j\right) f_{p_1} \otimes \cdots \otimes f_{p_N} = \left(|p_1|^2 + \cdots + |p_N|^2\right) \cdot f_{p_1} \otimes \cdots f_{p_N}$

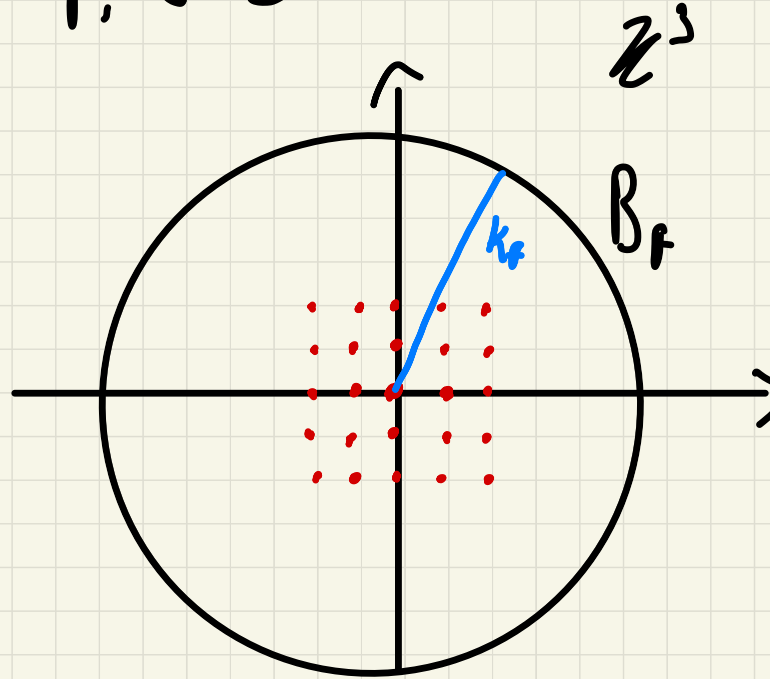
*) By lin, tensor prods are eigenvectors of $\sum_{j=1}^N -\Delta_j$

Ground state: choose $p_i \in \mathbb{Z}^3$ such that:

*) $p_i \neq p_j$ if $i \neq j$ $\qquad p_i \in \mathbb{Z}^3$

*) Minimize $\sum_i |p_i|^2$

*) From now on, B_F filled



$$N = \{ k \in \mathbb{Z}^3 \mid |k| \leq k_F \}$$

$$k_F = \left(\frac{3}{4\pi} \right)^{1/3} N^{1/3} + o(N^{1/3})$$

Kinetic en. of filled Fermi ball

$\forall \psi_N \in L^2_a(\mathbb{T}^{3N})$

$$\langle \psi_N, \sum_{i=1}^{N} -\Delta_i \psi_N \rangle \geq \sum_{k \in B_F} |k|^2$$

$$\sum_{k \in B_F} |k|^2 = N^{1+\frac{2}{3}} \sum_{k \in B_F} \frac{1}{N} |k|^2 \frac{1}{N^{2/3}}$$

$$\underset{N \gg 1}{\simeq} N^{5/3} \int_{|k| \leq \left(\frac{3}{4\pi}\right)^{1/3}} dk \, |k|^2 = \mathcal{O}(N^{5/3}) \gg \mathcal{O}(N)$$

More gen., $\forall\, \psi_N \in L^2_a(\mathbb{R}^{3N})$,

$$\Big(\psi_N, \sum_{j=1}^{N} -\Delta_j \psi_N\Big) \geq C_{LT} \int dx\, \rho_{\psi_N}(x)^{5/3}$$

$$\rho_{\psi_N}(x) = N \int dx_2 \dots dx_N\, |\psi(x, x_2, \dots, x_N)|^2$$

(density of particles at $x \in \mathbb{R}^3$)

<u>Lieb-Thirring kinetic energy inequality</u>

Mean field Hamiltonian:

$$H_N = \sum_{j=1}^{N} -\Delta_j + \frac{1}{N^{1/3}} \sum_{i<j}^{N} V(x_i - x_j)$$

Equivalently, setting $\varepsilon = N^{-1/3}$:

$$H_N = \sum_{j=1}^{N} -\varepsilon^2 \Delta_j + \frac{1}{N} \sum_{i<j}^{N} V(x_i - x_j)$$

Mean field + semiclassical scaling

Remark: We would like to argue that

$$\left\langle \psi_N, \frac{1}{N} \sum_{i<j}^{N} V(x_i - x_j) \psi_N \right\rangle$$

$$\simeq \frac{1}{2N} \int dx\, dy\, V(x-y)\, \rho_{\psi_N}(x)\, \rho_{\psi_N}(y)$$

<u>Law</u> of <u>large numbers</u>. ("density-density corr.")

*) Pauli principle introduces a correlation!

Hartree - Fock approximation.

Replace $L^2_a(\mathbb{T}^{3N})$ by :

$S_N = \{ f_1 \wedge f_2 \wedge \dots \wedge f_N \mid f_i$ ortho en $L^2(\mathbb{T}^3) \}$

= set of Slater dets.

Trivially, $S_N \subset L^2_a(\mathbb{T}^{3N})$ ("fermions possess nodes")

__Hartree-Fock__ ground __state__ energy:

$$E_N^{HF} = \inf_{\Psi_N \in S_N} \langle \Psi_N, H_N \Psi_N \rangle$$

Trivially, $E_N \leq E_N^{HF}$.

*) Advantage: $\langle \Psi_N, H_N \Psi_N \rangle$ is completely specified by the __reduced 1PDM__ of __Ψ_N__.

Def. Let $\psi_N \in L^2_a(\mathbb{R}^{3N})$. The k-part. reduced density matrix $\gamma^{(k)}$, $\gamma^{(k)} : L^2(\mathbb{R}^{3k}) \to L^2(\mathbb{R}^{3k})$

$$\gamma^{(k)}(x_1, \dots, x_k ; y_1, \dots, y_k) = \binom{N}{k} \int dz_{k+1} \dots dz_N \cdot$$

$$\cdot \psi_N(x_1, \dots, x_k, z_{k+1}, \dots, z_N) \cdot \overline{\psi_N(y_1, \dots, y_k, z_{k+1}, \dots, z_N)}$$

Rmk. Related to the notion of marginal in probab.

Rmk. $\gamma^{(k)}$ allows to compute average of k-pt ops. In particular:

$$(\psi_N, H_N \psi_N) = \mathrm{tr}_{L^2(\mathbb{R}^3)} \, (-\varepsilon^2 \Delta) \, \gamma^{(1)}_{\psi_N} + \frac{1}{N} \mathrm{tr}_{L^2(\mathbb{R}^6)} \, V(\hat{x}_1 - \hat{x}_2) \, \gamma^{(2)}_{\psi_N}$$

*) For a Slater det, $\gamma^{(1)} = \sum_{i=1}^{N} |f_i\rangle\langle f_i| =: \omega_N$ (ex.)

$\omega_N = \omega_N^2 = \omega_N^*$, $\mathrm{tr}\, \omega_N = N$.

All k part. density matrices can be comp. in terms of $\gamma^{(1)}$. [Wick's rule].

$\gamma^{(2)}(x_1, x_2; y_1, y_2) =$ [$\rho(x) = \omega(x,x)$

$= \frac{1}{2}\left[\omega(x_1, y_1)\,\omega(x_2, y_2) - \omega(x_1, y_2)\,\omega(x_2, y_1)\right]$

Hartree-Fock en. func. (= energy of Slater)

$\mathcal{E}_N^{HF}(\omega) = t_2 - \varepsilon^2 \Delta \omega + \frac{1}{2N}\int dx\,dy\, V(x-y)\Big[\rho(x)\rho(y) -$ (direct)

(exchange) $- |\omega(x,y)|^2 \Big]$

Rmks.

*) HF approx neglects correlations, except those due to antisym.

*) Trivial upper bd : $E_N \leq E_N^{HF}$.

Q: lower bd $E_N \geq E_N^{HF}$ − "small"

Recall: kinetic $O(N)$, direct $O(N)$,

exchange $\begin{cases} \text{bd } V & O(1) \\ \text{Coulomb} & O(N^{1/3}) \end{cases}$

Rigorous work. (Atoms, $Z \sim N \gg 1$)

*) Bach '92 $\quad E_N \geq E_N^{HF} - C N^{1/3-\alpha}$

$(\alpha > 0)$

*) Graf-Solovej '94 extension to jellium.

Def. (Correlation energy). We define:

$$E_N^c = E_N - E_N^{HF}.$$

Goal: get a better understanding of E_N^c.

__Rmk__ In general, E_N^{HF} is a complicated object.

*) Trivially, $E_N^{HF} \leq E_N^{Pr}$ (en. of the filled fermi ball $\psi_{p_1} \wedge \psi_{p_2} \dots \wedge \psi_{p_N}$)

$$\gamma(x,y) = \sum_{k \in B_F} \frac{e^{ik(x-y)}}{(2\pi)^3}$$ $\leftarrow |\psi_k\rangle\langle\psi_k|$

$$E_N^{Pr} = \sum_{k \in B_F} \varepsilon^2 |k|^2 + \frac{N}{2}\hat{V}(0) - \frac{1}{2N}\sum_{k,k' \in B_F} \hat{V}(k-k')$$

Prop. Let $\hat{V}(k) \in \ell^1(\mathbb{Z}^3)$, $\hat{V}(k) \geq 0$.

Then, $E_N^{pw} = E_N^{HF}$.

Rmk *) Uses that B_F is filled.

*) Not true, in gen (thermo limit).

For Jellium:

$$e^{HF}(\rho) - e^{pw}(\rho) \geq -C e^{-\rho^{1/6}}$$

| proven by: Gontier-Hainzl-Lewin 2018.

Thm (Main result) Let $\hat{V} \geq 0$, $(1+|k|)\hat{V} \in \ell^1$.

As $k_F \to \infty$:

$$E_N^c = E_N^{RPA} + \mathcal{O}(\varepsilon^{1+\alpha}) \qquad \alpha > 0, \quad \varepsilon = N^{-1/3}$$

$$E_N^{RPA} = \varepsilon \kappa_0 \sum_k |k| \left(\frac{1}{\pi} \int_0^{+\infty} \log\left(1 + 2\pi \kappa_0 \hat{V}(k)\left(1 - \lambda \arctan \frac{1}{\lambda}\right)\right) d\lambda - \frac{\pi}{2} \kappa_0 \hat{V}(k) \right), \quad \kappa_0 = \left(\frac{3}{4\pi}\right)^{1/3}$$

RPA = "Random Phase Approximation"

<u>Remarks</u>. | * methods are of rigorous <u>renormalization</u>.

* RPA introduced by Bohm-Pines '50s.

* HPR 18 : 2nd order result (V model)

* BNPSS 20-21 : V model, $\hat{V}$ comp. supp.

* BPSS 21 : this version

* CHN 21 : same res. diff. method

* CHN 22 : upper bound Coulomb.

Fermionic Fock space.

$$\mathcal{F} = \mathbb{C} \oplus \bigoplus_{n \geq 1} L^2_a(\mathbb{T}^{3n})$$

$$\mathcal{F} \ni \psi = (\psi^{(0)}, \psi^{(1)}, \dots, \psi^{(n)}, \dots)$$

$$\psi^{(n)} \in L^2_a(\mathbb{T}^{3n})$$

E.g.: $\Omega = (1, 0, 0, 0, \dots, 0, \dots)$

(no particles are present)

Creation / annihilation ops. :

Given $f \in L^2(\mathbb{T}^3)$, $\quad a(f) : \mathcal{F}^{(n)} \longrightarrow \mathcal{F}^{(n-1)}$

$a(f)\,\Omega = 0$. $\quad a^*(f) : \mathcal{F}^{(n)} \longrightarrow \mathcal{F}^{(n+1)}$

$$(a(f)\psi)^{(n)}(x_1,\dots,x_n) = \sqrt{n+1}\int dx\, \overline{f(x)}\,\psi^{(n+1)}(x, x_1,\dots,x_n)$$

$$(a^*(f)\psi)^{(n)}(x_1,\dots,x_n) = \frac{1}{\sqrt{n}}\sum_{j=1}^{n}(-1)^{j-1} f(x_j)\,\psi^{(n-1)}(x_1,\dots,\cancel{x_j},\dots,x_n)$$

Properties :

*) $a^*(f) = (a(f))^*$

$\{A, B\} = AB + BA$

*) Canonical Anticomm. Relations (CAR):

$$\{a(f), a(g)\} = \{a^*(f), a^*(g)\} = 0$$

$$\{a(f), a^*(g)\} = (f, g)_{L^2(\mathbb{R}^3)}$$

Consequence : $\quad \| a(g) \|_{\mathcal{F}} \leq \| g \|_2 \qquad \checkmark$

$$\| a^*(g) \|_{\mathcal{F}} \leq \| g \|_2 .$$

Check :

$$\langle \psi, a^*(g)\, a(g)\, \psi \rangle \qquad \left(= \| a(g) \psi \|^2 \right)$$

$$= \langle \psi, \{ a^*(g), a(g) \} \psi \rangle - \langle \psi, a(g)\, a^*(g) \psi \rangle$$

$$\leq \| g \|_2^2 \, \| \psi \|_{\mathcal{F}}^2 .$$

*) <u>Consequence</u> :

$$\langle f, \gamma^{(1)}_{\psi} f \rangle = \langle \psi, a^*(f)\, a(f)\, \psi \rangle$$

$$\leq \|f\|_2^2 \qquad \left(\|\psi\|_{\mathcal{F}} = 1 \right)$$

$$\Rightarrow \gamma^{(1)}_{\psi} \leq \mathbb{1}_{L^2(\mathbb{T}^3)} , \qquad \gamma^{(1)}_{\psi} \geq 0 .$$

[for bosons: $\gamma^{(1)}_{\psi} \leq N$] | $a^*_k = a^*(f_k)$

*) <u>Slater dets</u> : $f_{k_1} \wedge \dots \wedge f_{k_N} = a^*_{k_1} a^*_{k_2} \cdots a^*_{k_N} \Omega$

Rmk. $\{a^*_{k_1}\cdots a^*_{k_n}\Omega\}$ ONB of $\mathcal{F}$.

Lifting ops. on $\mathcal{F}$:

*) Consider: $\mathcal{N} := \bigoplus_{n\geq 0} n\,\mathbb{1}_{L^2(\mathbb{T}^{3n})}$

Claim: $\mathcal{N} = \sum_{k\in\mathbb{Z}^3} a^*_k a_k$.

$$a^*_k a_k a^*_{p_1}\cdots a^*_{p_n}\Omega \underset{k\notin\{p_i\}}{=} a^*_{p_1}\cdots a^*_{p_n}\overbrace{a^*_k a_k\Omega}^{=0}$$

Other case: $k \in \{p_i\}$ (can only appear once)

$$a_k^* a_k \, a_{p_1}^* \cdots a_k^* \cdots a_{p_n}^* \Omega =$$

$$= a_{p_1}^* \cdots a_{p_{n-1}}^* a_k^* \underbrace{a_k a_k^*}_{-\cancel{a_k^* a_k} + 1} \cdots a_{p_n}^* \Omega$$

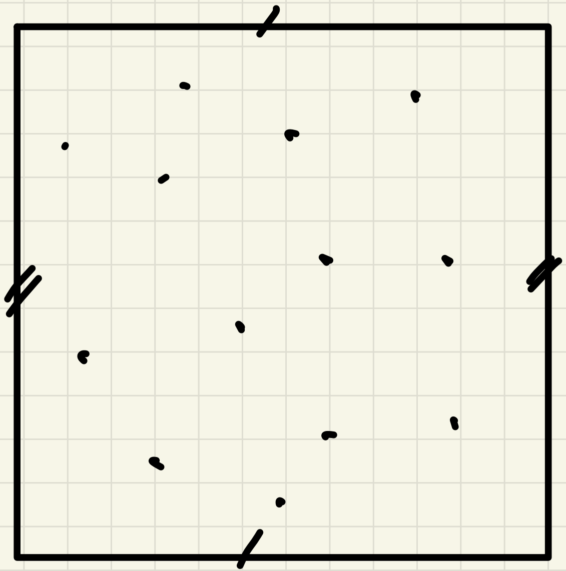
gives zero

$$= a_{p_1}^* \cdots a_k^* \cdots a_{p_n}^* \Omega$$

In conclusion,

$$N = \sum_{k \in \mathbb{Z}^3} a_k^* a_k$$

<u>Recap</u>: N interacting fermions on $\mathbb{T}^3$



$$H_N = \sum_{j=1}^{N} -\varepsilon^2 \Delta_j + \frac{1}{N} \sum_{i<j}^{N} V(x_i - x_j)$$

on $L^2_a(\mathbb{T}^{3N})$ $\quad (\varepsilon = N^{-1/3})$

Correlation energy:

$$E_N^c := E_N - E_N^{HF}$$

We are interested in computing E_N^c as $N \to \infty$

Recap :

$$\psi = (\psi^{(0)}, \psi^{(1)}, \dots, \psi^{(n)}, \dots)$$

* Fock space $\mathcal{F} = \mathbb{C} \oplus \bigoplus_{n\geq 1} L^2_a(\mathbb{T}^{3n})$

* Creation/annihilation ops a^*_k, a_k

$$\{a_k, a^*_q\} = \delta_{kq}, \quad \{a_k, a_q\} = \{a^*_k, a^*_q\} = 0$$

basis of $\mathcal{F}$: $\{a^*_{k_1} \dots a^*_{k_n} \Omega\}$ $\quad k_i \in \mathbb{Z}^3$

* lifting of ops on $\mathcal{F}$:

$$\mathcal{N} = \bigoplus_{n\geq 0} n \mathbb{1}_{L^2(\mathbb{T}^{3n})} = \sum_k a^*_k a_k$$

Similarly, $K = \bigoplus_{n\geq 0} \sum_{j=1}^{n} -\varepsilon^2 \Delta_j = \sum_{k\in\mathbb{Z}^3} \varepsilon^2 |k|^2 a_k^* a_k$

Finally, the many body Hamiltonian is:

$$\mathcal{H}_N = \bigoplus_{n\geq 0} H_N^{(n)}$$

$$= \sum_k \varepsilon^2 |k|^2 a_k^* a_k + \frac{1}{2N} \sum_{p,q,k} \hat{V}(k)\, a_{p+k}^* a_{q-k}^* a_q a_p$$

Ground state energy: || Compare with $\underline{E_0^{HF} = E_N^{HF}}$

$$E_N = \inf_{\psi\in\mathcal{F}^{(N)},\ \|\psi\|=1} \langle \psi, \mathcal{H}_N \psi \rangle .$$

Bogoliubov transformations

$\Omega = (1, 0, 0 \ldots)$

$\exists\, R : \mathcal{F} \to \mathcal{F}$ unitary such that:

a) $R\,\Omega = \left[\prod_{k \in B_F} a^*_k\right] \Omega$ (free Fermi gas)

b) $R\, a^*_p\, R^* = \begin{cases} a^*_p & p \notin B_F \\ a_p & p \in B_F \end{cases}$ (particle-hole transform.)

[the prop. actually define the map.]

Energy of free Fermi gas:

$$E_N^{FG} = \langle R\Omega, H_N R\Omega \rangle = \langle \Omega, R^* H_N R \Omega \rangle$$

More generally, for any $\psi \in \mathcal{F}$:

$$E(\psi) = \langle \overset{RR^*}{\downarrow}\psi, H_N \overset{RR^*}{\downarrow}\psi \rangle = \langle R^*\psi, R^* H_N R R^* \psi \rangle$$

Remarks: If $\psi \simeq \psi_{gs}$, expect $R^*\psi$ to have "few particles"

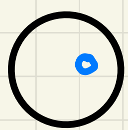
It is useful to compute $R^* H R$

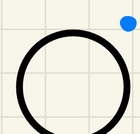
Test run : number operator.

$$R^* \mathcal{N} R = \sum_k R^* a_k^* \underset{\nwarrow R R^*}{} a_k R$$

$$= \sum_{k \in B_F} \underbrace{a_k a_k^*}_{= 1 - a_k^* a_k} + \sum_{k \notin B_F} a_k^* a_k$$

$$= \underset{\nearrow \langle \Omega, \mathcal{N} \Omega \rangle}{\overset{=}{N}} - \underbrace{\sum_{k \in B_F} a_k^* a_k}_{=: \mathcal{N}_h} + \underbrace{\sum_{k \notin B_F} a_k^* a_k}_{=: \mathcal{N}_p}$$





Rmk: $\mathcal{N}\psi = N\psi \iff (\mathcal{N}_p - \mathcal{N}_h) R^*\psi = 0$

* Similarly, for the kinetic energy:

$$R^* K R = \sum_{k \in B_F} \varepsilon^2 |k|^2 + \sum_{k \notin B_F} \varepsilon^2 |k|^2 a_k^* a_k$$

$$- \sum_{k \in B_F} \varepsilon^2 |k|^2 a_k^* a_k \qquad [\mu = \varepsilon^2 k_F^2$$

$\langle R\Omega, KR\Omega \rangle \rightsquigarrow$

$$= \sum_{k \in B_F} \varepsilon^2 |k|^2 + \sum_k e(k) a_k^* a_k$$

where $e(k) = |\varepsilon^2 |k|^2 - \mu|$ [add $\mu(\mathcal{N}_h - \mathcal{N}_p)$]

Correlation Hamiltonian: for $\mathcal{N}\psi = N\psi$,

$$\langle \psi, \mathcal{H}_N \psi \rangle = \underbrace{E_N^{\mathrm{pw}}}_{\langle R\Omega,\, \mathcal{H}_N R\Omega\rangle} + \langle R^*\psi, \underbrace{\mathcal{H}_N^{\mathrm{corr}}}_{\text{corr. Ham.}} R^*\psi \rangle$$

* In particular, the correlation energy is

$$E_N^{c} = \inf_{\substack{\xi \in \mathcal{X}(\mathcal{N}_p - \mathcal{N}_h = 0) \subset \mathcal{F} \\ \|\xi\| = 1}} \langle \xi, \mathcal{H}_N^{\mathrm{corr}} \xi \rangle$$

Rmk. ξ are not eigenstates of $\mathcal{N}$!

In order to estimate $\mathcal{H}_N^{\text{corr}}$, need a priori estim.

Prop. Let $\hat{V} \geq 0$, $(1+|k|)\hat{V} \in L^1$, $\mathcal{N}\psi = N\psi$.

Suppose $\langle \psi, H\psi \rangle \leq E_N^{\text{HF}}$. Then:

$$\langle R^*\psi, \mathbb{H}_0 R^*\psi \rangle \leq C\varepsilon \qquad (\varepsilon = N^{-1/3})$$

and

$$\langle R^*\psi, \mathcal{N} R^*\psi \rangle \leq C N^{1/3}$$

Recall:

$\mathbb{H}_0 = \sum_k e(k) a_k^* a_k$

$e(k) = |\varepsilon^2 |k|^2 - \mu|$

Proof: From $\hat{V}(k) \geq 0$: | $\boxed{\geq 0}$

$$\int \mu(dx)\,\mu(dy)\,V(x-y) = \sum_k \hat{V}(k)\,\left|\mu(e^{ik\cdot x})\right|^2$$

Choose: $\mu(dx) = dx\left(\sum_{j=1}^{N} \delta(x_j - x) - \frac{N}{(2\pi)^3}\right)$

$$\sum_{i,j=1}^{N} V(x_i - x_j) - \underbrace{2\sum_{i=1}^{N} \int dy\, V(x_i - y)\,\frac{N}{(2\pi)^3} + N^2\,\hat{V}(0)}_{-N^2\hat{V}(0)} \geq 0$$

$$\Rightarrow \sum_{i<j}^{N} V(x_i - x_j) \geq \frac{N^2}{2}\hat{V}(0) - \frac{N}{2}V(0)$$

<u>Therefore</u>: $\quad (\|\psi\| = 1)$

$$\langle \psi, H\psi \rangle \geq \langle \underset{\substack{\uparrow \\ RR^*}}{\psi}, K \underset{\substack{\uparrow \\ RR^*}}{\psi} \rangle + \frac{N}{2}\hat{V}(0) - \frac{1}{2}V(0)$$

$\mathcal{N}\psi = N\psi$

$$\searrow \; = \underbrace{\sum_{k \in B_F} \varepsilon^2 |k|^2 + \frac{N}{2}\hat{V}(0) - \frac{1}{2}V(0)}_{(E_N^{HF})} + \langle R^*\psi, \mathbb{H}_0 R^*\psi \rangle .$$

<u>Claim</u>:

$$\geq E_N^{HF} - C\varepsilon + \langle R^*\psi, \mathbb{H}_0 R^*\psi \rangle$$

In fact: $E_N^{GS} = E_N^{HF}$

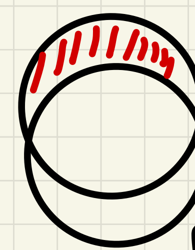
$$= \sum_{k\in B_F} \varepsilon^2 |k|^2 + \frac{N}{2}\hat{V}(0)$$

$$- \frac{1}{2N}\sum_{q,k}\hat{V}(q)\,\chi_{B_F}(k)\,\chi_{B_F}(k+q)$$

$$*) \quad -\frac{1}{2}V(0) \geq -\frac{1}{2N}\sum_{q,k}\hat{V}(q)\,\chi_{B_F}(k)\,\chi_{B_F}(k+q)$$

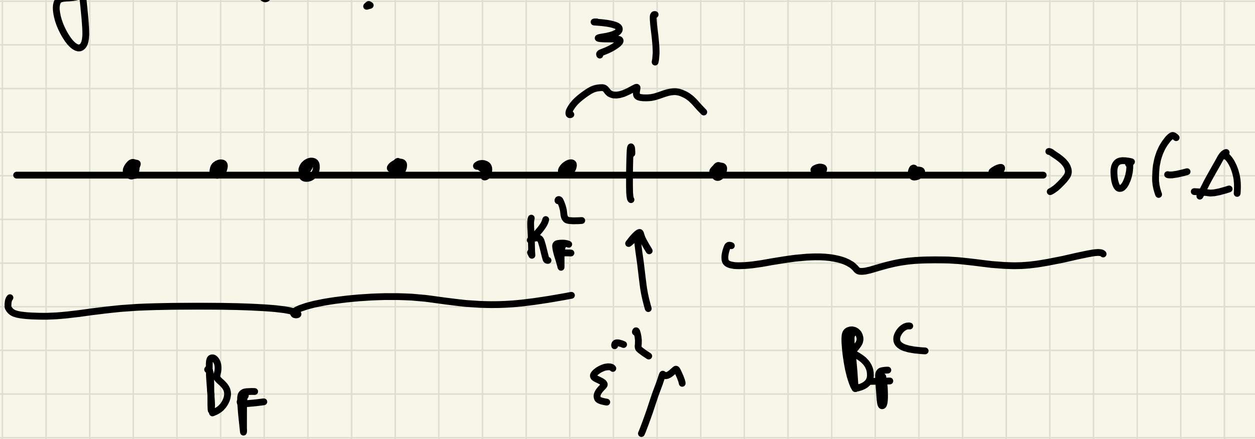
$$-C\varepsilon$$

$\mathcal{O}(N^{2/3}|q|)$



$$\Rightarrow \langle \mathfrak{R}^* \psi, \mathbb{H}_0 \mathfrak{R}^* \psi \rangle \le C \varepsilon . \qquad \checkmark$$

Bound for $\mathcal{N}$?



$$\Rightarrow \left| \varepsilon^2 |k|^2 - \mu \right| \ge \frac{\varepsilon^2}{2} \quad \Rightarrow \quad \mathbb{H}_0 \ge \frac{\varepsilon^2}{2} \mathcal{N} \qquad \blacksquare$$

<u>Rmk</u>. $\langle R^* \psi, \mathcal{N} R^* \psi \rangle$ useful to estimate diff. between states.

$$\langle R^* \psi, \mathcal{N} R^* \psi \rangle = \langle \psi, (N - \mathcal{N}_p + \mathcal{N}_u) \psi \rangle$$

$$= 2 \operatorname{tr}_2 \gamma_\psi (1 - \omega) \quad (\text{ex.})$$

$$\operatorname{tr}_2 |\gamma_\psi^{(1)} - \omega|^2 \le \operatorname{tr}_2 \left[\gamma_\psi^{(1)} + \omega - 2 \omega \gamma_\psi^{(1)} \right]$$

$$= 2 \operatorname{tr}_2 \gamma_\psi^{(1)} (1 - \omega)$$

Back to the correlation Hamiltonian:

$$R^* H R = E_N^{pw} + \mathcal{H}_N^{corr} \quad \text{on } \mathcal{X}(\mathcal{N}_p - \mathcal{N}_h = 0)\mathcal{F}$$

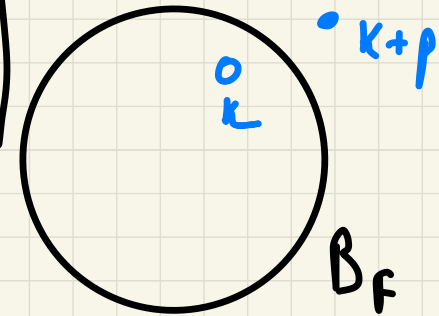
with: $$\mathcal{H}_N^{corr} = \mathbb{H}_0 + \underbrace{\mathbb{Q} + \mathcal{E}_1 + \mathcal{E}_2 + \mathbb{X}}_{\text{arising from } R^* V R}$$

Recall: $$V = \frac{1}{2N} \sum_{p,k,q} \hat{V}(p)\, a^*_{k+p}\, a^*_{q-p}\, a_q\, a_k$$

and $$R^* a_k R = \begin{cases} a_k & k \notin B_F \\ a^* & k \in B_F \end{cases}$$

Main term: particle/hole exc. around ∂B_F

$$Q = \frac{1}{2N} \sum_p \hat{V}(p) \left[2 b_p^* b_p + b_p^* b_{-p}^* + b_{-p} b_p \right]$$



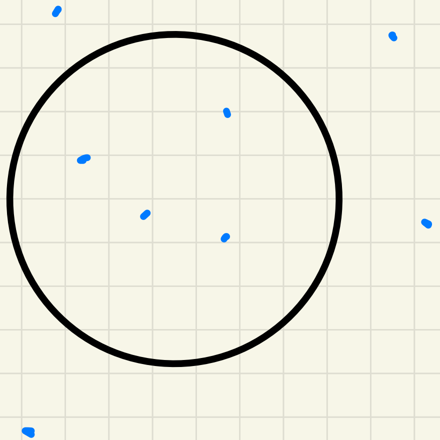
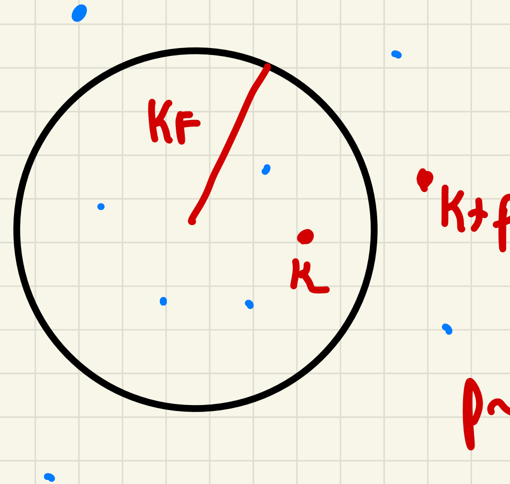
$$b_p = \sum_{\substack{k:\, k+p \notin B_F \\ k \in B_F}} a_{k+p}\, a_k$$

Other: (ex.)

$$\mathcal{E}_1 = \frac{1}{2N} \sum_p \hat{V}(p)\, D_p^* D_p \, ,$$

$$D_p = \sum_{\substack{k+p \notin B \\ k \notin B}} a_{k+p}^* a_k - \sum_{\substack{k-p \in B \\ k \in B}} a_{k-p}^* a_k$$

The Q term is "bosonic":

b_p^*  $= \sum_k$ 

$p \sim 1$

$k_F \sim N^{1/3}$

"pairs of fermions" $\approx$ "bosons"

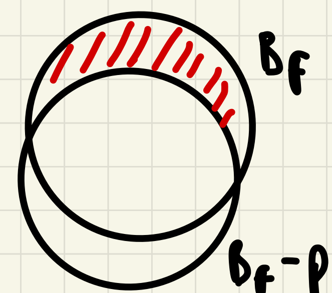
Approximate CCR:

$\mathcal{E}(\psi) \le \mathcal{E}^{HF}_{N}$

$\langle \mathcal{R}^* \psi, \mathcal{N} \mathcal{R}^* \psi \rangle \le C N^{1/3}$

*) $[b_p, b_q] = [b_p^*, b_q^*] = 0$

*) $[b_p, b_q^*] \overset{\text{ex.}}{=} \underbrace{\delta_{pq} \sum_{\substack{k : k+p \notin B \\ k \in B}} 1}_{\mathcal{O}(|p| N^{2/3})} + \text{"}\mathcal{O}(\mathcal{N})\text{"}$



$\Rightarrow$ the error term is subleading, "close" to g.s.

Rmk: After renormaliz., b_p, b_q^* behave as "bosons".

Hence, $H_N^{\text{ren}} = \mathbb{H}_0 + Q + (\text{"small"})$

quadratic in a, a^* quadratic in b, b^*

<u>Hope</u>: in middle range, $\mathbb{H}_0$ can be approx by a quad. op. in b, b^* (?)

<u>Eg</u>: $[\mathbb{H}_0, b_p^*]$ is approx. linear in b, b^* (!)

$$[\mathbb{H}_0, b_p^*] = \sum_k e(k) \sum_{\substack{k' : k'+p \notin B_F \\ k' \in B_F}} [a_k^* a_k, a_{k'+p}^* a_{k'}^*]$$

$$= \sum_{\substack{k \\ k'+p \notin B_F,\, k' \in B_F}} e(k)\, a_{k'+p}^* a_{k'}^* \left(\delta_{k,k'+p} + \delta_{k,k'} \right)$$

$$= \sum_{\substack{k:\, k+p \notin B_F \\ k \in B_F}} \big(e(k+p) + e(k) \big) a^*_{k+p} a^*_{k} \qquad (*)$$

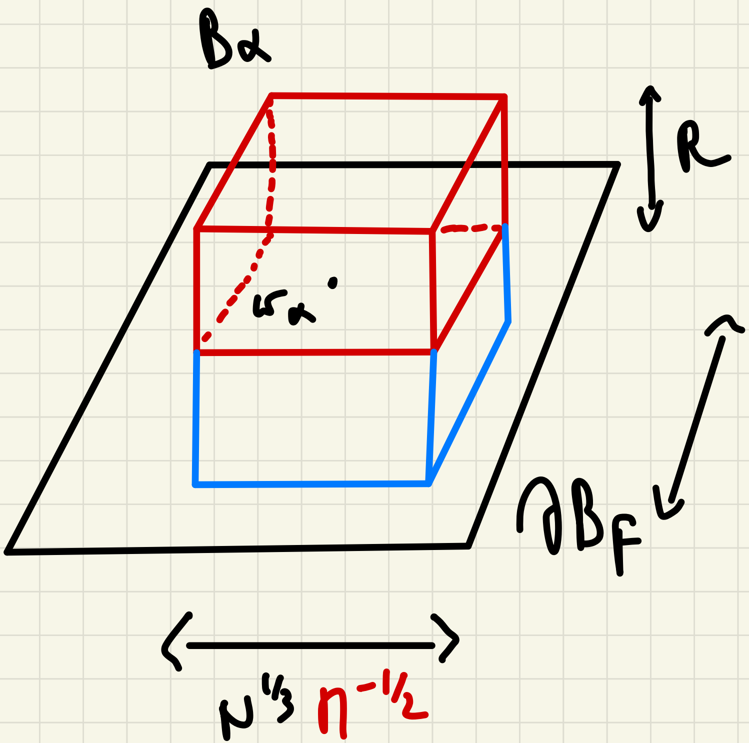
$$e(k+p) + e(k) = \varepsilon^2 |k+p|^2 - \mu + \mu - \varepsilon^2 |k|^2$$

$$= \underbrace{2\varepsilon^2 k \cdot p}_{\mathcal{O}(\varepsilon)} + \underbrace{\varepsilon^2 |p|^2}_{\mathcal{O}(\varepsilon^2)}$$

* Not linear in b, b^* !
* If $k \cdot p \to \omega \cdot p$ then $(*) \simeq \lambda_p b^*_p$!

Patching of the Fermi surface.

Find "better" bosonic variables.



$\hat{V}(k) = 0 \quad |k| > R = O(N^{\gamma})$

$M = O(N^{\delta}) \quad \delta > 0$

$N^{1/3} M^{-1/2}$

B_α = "thick patch"

Basis area:

$\frac{4\pi}{M} k_F^2 (1 + o(1))$

Define the "local boson":

$$b_\alpha(p) = \sum_{\substack{k+p \in B_F^c \cap B_\alpha \\ k \in B_F \cap B_\alpha}} \frac{a_{k+p}\, a_k}{n_\alpha(p)}$$

s.t. : $\| b_\alpha^*(p)\, \Omega \| = 1$ $\left[n_\alpha(p)^2 = \frac{4\pi k_F^2}{M} |p \cdot \hat{\omega}_\alpha| \left(1+o(1)\right) \right]$

$$* \left[\mathbb{H}_0, b_\alpha^*(p) \right] = \frac{1}{n_\alpha(p)} \sum_{\substack{k+p \in B_F^c \cap B_\alpha \\ k \in B_F \cap B_\alpha}} \left(2\varepsilon^2 \left(k - \omega_\alpha + \omega_\alpha\right) \cdot p + \varepsilon^2 |p|^2 \right) a^*_{k+p}\, a^*_k$$

<u>But</u>: $\| k - \omega_\alpha \| \sim N^{1/3} M^{-1/2} \ll \| \omega_\alpha \|$!

Therefore, for M large enough:

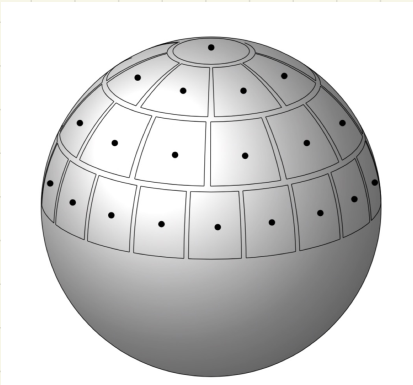
$$[\mathbb{H}_0, b^*_\alpha(p)] = 2\varepsilon |p| \cdot |\hat{\omega}_\alpha \cdot \hat{p}| \, b^*_\alpha(p) + \text{small}$$

* Neglecting the errors, it agrees with:

$$\left[2\varepsilon |p| \, d_\alpha(p) \, b^*_\alpha(p) b_\alpha(p), \, b^*_\alpha(p) \right]$$

with $d_\alpha(p) = |\hat{\omega}_\alpha \cdot \hat{p}|$

Covering of Fermi surface with patches



$B_\alpha \quad , \quad \alpha = 1, \ldots, M$

$(M = \mathcal{O}(N^\alpha))$

$\mathrm{diam}\,(B_\alpha, B_{\alpha'}) = R$

RmK : need $n_\alpha(p)$ to be large

$\left[n_\alpha(p) \simeq \frac{4\pi k_F^2}{M} |p \cdot \omega_\alpha| \right]$

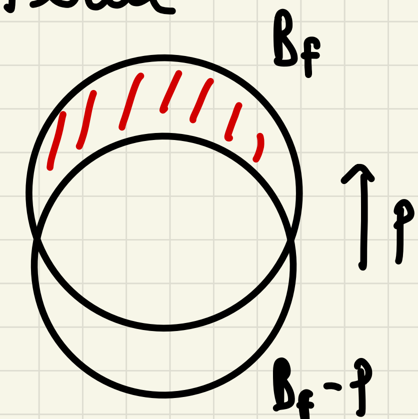
Admissible patches :

$I_p^+ = \{ \alpha \mid k \cdot \omega_\alpha \geq N^{-\delta} \}$

$I_p^- = \{ \alpha \mid k \cdot \omega_\alpha \leq -N^{-\delta} \}$

Decomposition of "global bosons":

$$b_p = \sum_{\alpha \in I_p^+} n_\alpha(p)\, b_\alpha(p) + \text{error term}$$



$(b_{-p} \to I_p^-)$.

Define:

$$c_\alpha(p) = \begin{cases} b_\alpha(p) & \alpha \in I_p^+ \\ b_\alpha(-p) & \alpha \in I_p^- \end{cases}$$

$$[c_\alpha(k), c_\alpha(p)] = 0$$

$$[c_\alpha(k), c^*_\beta(p)] = \delta_{\alpha\beta}(\delta_{k\ell} + \mathcal{E}_\alpha)$$

$$\mathcal{E}_\alpha \sim M N^{-2/3+\delta}$$

To summarize:

* $\mathbb{Q} = \frac{1}{2N} \sum_p \hat{V}(p) \left(2 b_p^* b_p + b_p^* b_{-p}^* + b_{-p} b_p \right)$

can be decomp. into "local bosons" ($c_\alpha(p)$)

$$\mathbb{Q} = \mathbb{Q}_B + \text{small (on the g.s.)}$$

* $[\mathbb{H}_0 - \mathbb{D}_B, c_\alpha(p)]$ is small (on the g.s.)

$$\mathbb{D}_B = \sum_{\alpha, p} 2\varepsilon |p|\, d_\alpha(p)\, c_\alpha^*(p)\, c_\alpha(p) \qquad \left(d_\alpha(p) = |\hat{\omega}_\alpha \cdot \hat{p}| \right)$$

For two bosons, $\mathcal{H}_B = \mathbb{D}_B + Q_B$ could be block-diag. via a Bosonic Bog. transfo:

$$T^* \mathcal{H}_B T = E_N^{RPA} + \sum_p \sum_{\alpha\beta} \varepsilon(k)\, c_\alpha^*(p)\, h_{\alpha\beta}^{exc}(k)\, c_\beta(p)$$

with $T = \exp\left(\sum_p \sum_{\alpha\beta} c_\alpha^*(p)\, c_\beta^*(p)\, K_{\alpha\beta}(p) - h.c.\right)$

for a suitable Bog. kernel $K_{\alpha\beta}(p)$

(of order $\hat{V}(p)/M$)

However, $\mathcal{H}_N^{com} \neq \mathcal{H}_B$! In particular,

$\mathbb{H}_0 \simeq \mathbb{D}_B$ only in a "commutator sense"

Idea : let $\xi = R^* \psi$ with ψ "close" to the ground state $\left(\mathcal{E}(\psi) \simeq E_N^{HF} \right)$.

$$\mathcal{E}(\psi) = E_N^{HF} + \langle \xi, (\mathbb{H}_0 + \mathbb{Q}_B) \xi \rangle + \text{"small"}$$

$$= E_N^{HF} + \langle \xi, \underbrace{(\mathbb{H}_0 - \mathbb{D}_B)}_{(\mathrm{I})} \xi \rangle + \overbrace{\langle \xi, (\mathbb{D}_B + \mathbb{Q}_B) \xi \rangle}^{(\mathrm{II})} \; (+ \text{ small})$$

$$\mathrm{II.}\ \langle \xi, (\mathbb{D}_B + Q_B)\xi \rangle =$$

$$= \langle T^*\xi, T^*(\mathbb{D}_B + Q_B) T T^*\xi \rangle$$

$$= E_N^{\mathrm{RPA}} + \underbrace{\langle T^*\xi, H_N^{\mathrm{exc}} T^*\xi \rangle}_{\geq 0}$$

$\underline{\mathrm{Rmk}}$: $\langle T^*\xi, H_N^{\mathrm{exc}} T^*\xi \rangle = 0$ if $\xi = T\Omega$.

(ok for trial state)

$\mathrm{I}. \quad \langle \xi, (\mathbb{H}_0 - \mathbb{D}_B)\xi \rangle$

$$= \langle T^*\xi, (\mathbb{H}_0 - \mathbb{D}_B) T^*\xi \rangle \quad (+\text{ small})$$

For the <u>upper bound</u>, $T^*\xi = \Omega \Rightarrow \mathrm{I} = 0$!

<u>Lower bound</u> : $-\mathbb{D}_B$ is not positive!

<u>Idea</u>: use positivity of $\mathbb{H}_D^{exc}$ to control $-\mathbb{D}_B$.

* For small V, $H_B^{exc} = \mathbb{D}_B +$ "$\mathcal{O}(\hat{V}\,\mathbb{H}_0)$"
(as in BNPSS21)

* To relax smallness cond. on V, we use a second bosonic Bog. transfo, $\left[\mathcal{Z}^*(\mathbb{H}_0 - \mathbb{D}_B)\mathcal{Z} \simeq (\mathbb{H}_0 - \mathbb{D}_B) \right.$ and show:

$$\mathcal{Z}^* H_B^{exc} \mathcal{Z} \gtrsim \mathbb{D}_B - o(\varepsilon)$$

Remarks:

* Bosonization introduced by Mattis-Lieb ('60s)

* Application to $d>1$ cond. mat. systems:
(nonrig.) Luther (late 70s), Haldane ('90s) ...

* Patches = sectors in RG community:
Benfatto-Gallavotti; Feldman-Knörrer-Trubowitz-Salmhofer ... ;

* Patch-free approach: Christiansen, Hainzl, Nam '21